

Amendments to the Claims:

This listing of claims will replace all prior versions and listings of claims in the application.

Listing of Claims:

1. (Currently Amended) A crystal of BTK kinase domain of SEQ ID NO:4 having a space group symmetry of $P2_12_12_1$ and ~~comprising~~ a unit cell having the dimensions of a , b , and c , where a is ~~about~~ 45 Å, b is ~~about~~ 104 Å, and c is ~~about~~ 116 Å.
2. (Currently Amended) The crystal of claim 1, having ~~an amino acid sequence of~~ SEQ ID NO:4 the structural coordinates listed in Table 1.
3. (Withdrawn) A molecule or molecular complex comprising at least a portion of the BTK kinase domain binding pocket, wherein the binding pocket comprises the amino acids listed in Table 2, the binding pocket defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.
4. (Withdrawn) A scalable three-dimensional configuration of points, at least a portion of said points derived from structure coordinates listed in Table 1, comprising a BTK kinase domain binding pocket, wherein the BTK kinase domain forms a crystal having the space group symmetry $P2_12_12_1$.
5. (Withdrawn) The scalable three-dimensional configuration of points of claim 4, wherein substantially all of the points are derived from structure coordinates listed in Table 1.

6. (Withdrawn) The scalable three-dimensional configuration of points of claim 4, wherein at least a portion of the points are derived from structure coordinates representing locations of at least the backbone atoms of amino acids defining the BTK kinase domain binding pocket.

7. (Withdrawn) The scalable three-dimensional configuration of points of claim 4, wherein the binding pocket comprises the amino acids listed in Table 2.

8. (Withdrawn) A scalable three-dimensional configuration of points displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image, at least a portion of said points derived from structure coordinates listed in Table 1, comprising a BTK kinase domain binding pocket, wherein the BTK kinase domain forms a crystal having the space group symmetry $P2_12_12_1$.

9. (Withdrawn) A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein a machine programmed with instructions for using such data displays a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a BTK kinase domain binding pocket, the binding pocket defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of said amino acids as represented by the structure coordinates listed in Table 1.

10. (Withdrawn) A machine readable data storage medium comprising data storage material encoded with a first set of machine readable data which is combined with a second set of machine readable data using a machine programmed with instructions for using said first and second sets of data, determines at least a portion of the structure coordinates corresponding to the second set of data, wherein the first set of data comprises a Fourier transform of at least a portion of the BTK kinase domain structural coordinates of Table 1, and wherein the second set of data comprises an X-ray diffraction pattern of an unknown molecule or molecular complex.

11. (Withdrawn) A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the BTK kinase domain structure coordinates of Table 1 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

12. (Withdrawn) A computer-assisted method for identifying an agent that modulates BTK activity comprising:

- (a) providing a computer modeling application with a set of structure coordinates of Table 1 defining at least a portion of a BTK kinase domain;
- (b) providing the computer modeling application with a set of structure coordinates for a test compound; and
- (c) modeling the structure of (a) complexed with (b) to determine if the test compound binds to the BTK kinase domain binding pocket.

13. (Withdrawn) The method of claim 12, where the binding pocket comprises the amino acids listed in Table 2.

14. (Withdrawn) A computer-assisted method for designing a compound that binds the BTK kinase domain binding pocket, comprising:

- (a) providing a computer modeling application with a set of structural coordinates of Table 1 defining at least a portion of the BTK kinase domain; and
- (b) modeling the structural coordinates of (a) to determine a complementary molecule that binds the BTK kinase domain pocket.

15. (Withdrawn) A molecular complex comprising a BTK kinase domain binding pocket defined by at least a portion of the structural coordinates of Table 1 complexed with a compound having complementarity to at least a portion of the structural coordinates of Table 1.

16. (New) A method for identifying a compound that modulates BTK activity comprising:
using the structure coordinates of the crystal of claim 2 and listed in Table 1 to construct a model of the crystal including the BTK kinase domain binding pocket; and
designing a compound that complements the crystal's BTK kinase domain binding pocket.

17. (New) A method for identifying a compound that modulates BTK activity comprising:
providing the atomic coordinates of the crystal of claim 2; and
using the atomic coordinates of the crystal and a molecular modeling technique to identify a compound that interacts with a portion of the BTK kinase domain defined by the coordinates.

18. (New) The method according to claim 17 further comprising:
assaying the identified compound for modulation of BTK kinase activity.

19. (New) A method for modeling BTK homolog activity comprising:
creating a first model of a BTK homolog by aligning the sequence of a BTK homolog with the sequence of the BTK kinase domain crystal of claim 1; and
minimizing the energy of the first model to yield an energy minimized model of the BTK homolog.

20. (New) A method for preparing a crystal of the BTK kinase domain of claim 1 comprising:
preparing a purified BTK kinase domain; and
crystallizing the BTK kinase domain from a solution comprising the purified BTK kinase domain, polyethylene glycol, Tris/HCl, and DTT, the solution being buffered at a pH of about 8.0.

21. (New) A crystal of the BTK kinase domain of claim 1 prepared by the process of claim 20.